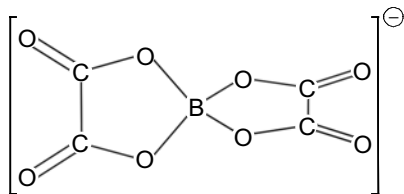


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Structural Chemistry of Novel *Bis*(Oxalato)Borate Salts and Their Solvates. Peter Y. Zavalij, M. Stanley Whittingham, Institute for Materials Research & Chemistry Dept., Binghamton Univ. (SUNY), Binghamton, NY 13902, USA.

Recently, in attempt to replace fluorine or arsenic containing lithium salts, which are currently in use as a source of conducting lithium ions in the battery electrolytes, the new safer lithium *bis*(oxalato)borate (BOB), $\text{LiB}(\text{C}_2\text{O}_4)_2$, is being explored.



However, the crystal structure of any BOB compounds was unknown. This work presents structural studies using powder and single crystal methods of 11 BOB compounds: anhydrous *MBOB* ($M=\text{Li,Na,K}$), solvates with water ($\text{LiBOB}\cdot\text{H}_2\text{O}$), acetonitrile ($2\text{LiBOB}\cdot 5\text{AN}$), acetone ($3\text{LiBOB}\cdot 4\text{AC}$), dimethoxyethane ($\text{LiBOB}\cdot\text{DME}$), 1,3-dioxolane ($2\text{LiBOB}\cdot 3\text{DO}\cdot\text{H}_2\text{O}$), as well as ethylenecarbonate Li complexes $[\text{Li}(\text{EC})_4]^+$ with BOB^- , PF_6^- , and

AsF_6^- ions. The coordination polyhedra of Li are: square pyramid in anhydrous salt, octahedra in solvates and tetrahedra in *EC* complexes. Interestingly, among all studied solvents only *EC* forms tetrahedral cationic complex which could help to explain why mainly this solvent is used in the battery electrolytes.

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